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SESSION RESUMED IN FILE 'HOME' AT 11:48:35 ON 04 MAR 2008

FILE 'HOME' ENTERED AT 11:48:35 ON 04 MAR 2008

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 11:48:44 ON 04 MAR 2008

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 3 MAR 2008 HIGHEST RN 1006431-93-1

DICTIONARY FILE UPDATES: 3 MAR 2008 HIGHEST RN 1006431-93-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\zaswer.str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Updated Search

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 11:54:00 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 2 TO 124
PROJECTED ANSWERS: 2 TO 124

L2 2 SEA SSS SAM L1

=> s l1 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 11:54:05 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 18 TO ITERATE

100.0% PROCESSED 18 ITERATIONS 13 ANSWERS
SEARCH TIME: 00.00.01

L3 13 SEA SSS FUL L1

=> s l3 and takada, y?/au

NUMERIC VALUE NOT VALID 'TAKADA, Y?'

0 TAKADA, Y?/AU

L4 0 L3 AND TAKADA, Y?/AU

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	188.11	188.32

FILE 'HCAPLUS' ENTERED AT 11:55:37 ON 04 MAR 2008

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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FILE COVERS 1907 - 4 Mar 2008 VOL 148 ISS 10

FILE LAST UPDATED: 3 Mar 2008 (20080303/ED)

Updated Search

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

L5 180 L3

=> s 13/prep

180 L3

4537224 PREP/RL

L6 10 L3/PREP

(L3 (L) PREP/RL)

=> s 16 and takada, y?/au

2785 TAKADA, Y?/AU

L7 1 L6 AND TAKADA, Y?/AU

=> d 17, ibib abs hitstr, 1

L7 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:324169 HCAPLUS

DOCUMENT NUMBER: 142:392537

TITLE: Process for producing optically active dihydropyridinephosphonic ester by crystallization of racemate using optically active seed crystals

INVENTOR(S): Takada, Yasutaka; Matsumoto, Hiroo

PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 21 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005033117	A1	20050414	WO 2004-JP11607	20040812
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1676852	A1	20060705	EP 2004-771582	20040812
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR			
US 2006276437	A1	20061207	US 2006-573972	20060330
PRIORITY APPLN. INFO.:			JP 2003-342761	A 20031001
			WO 2004-JP11607	W 20040812

OTHER SOURCE(S): MARPAT 142:392537

AB There is provided an economical process for efficiently producing an optically active isomer of efonidipine (I), the isomer being useful as an

Updated Search

antihypertensive agent or a therapeutic agent for angina pectoris. The above process for producing an optically active isomer of the compound I is characterized in that a racemate of the compound I is dissolved in a solvent to prepare a supersatd. solution and crystals of one of the optically active isomers of the compound I are added as seed crystals to the supersatd. solution to precipitate crystals of the optically active isomer whose seed crystals were added, or that a mixture of optically active isomers of the compound I in which either of the isomers is present in excess is dissolved in a solvent to prepare a supersatd. solution and crystals of the optically active isomer which is present in excess are added as seed crystals to the supersatd. solution to precipitate crystals of the optically active isomer present in

excess.

Thus, 1.00 g racemic I was dissolved in 25.0 g MeOH at 62°, cooled to 53° over 20 min, seeded with 10 mg (S)-(+)-I (100% ee), cooled to 33° over 45 min, and stirred at 30-33° for 1 h. The precipitated crystals were collected by filtration and dried at 50° under reduced pressure to give 144.8 mg (S)-(+)-I (88.37% ee) as light yellow crystal. The filtrate was concentrated to give 771.6 mg (R)-(-)-I (13.33% ee) as a yellow foam.

IT 128194-12-7P, (S)-(+)-Efonidipine 128194-13-8P,
(R)-(-)-Efonidipine

RL: IMF (Industrial manufacture); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)

(process for producing optically active (S)-(+)-efonidipine as antihypertensive by crystallization of racemate from supersatd. solution

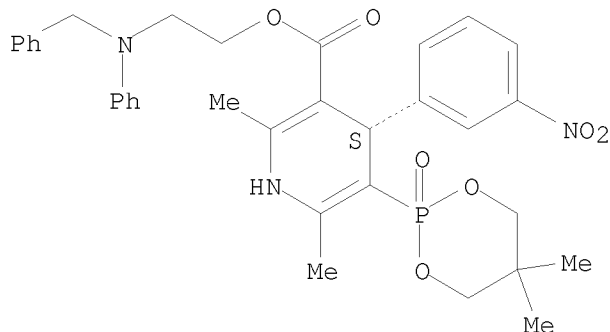
using

optically active seed crystals)

RN 128194-12-7 HCAPLUS

CN 3-Pyridinecarboxylic acid, 5-(5,5-dimethyl-2-oxido-1,3,2-dioxaphosphorinan-2-yl)-1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-, 2-[phenyl(phenylmethyl)amino]ethyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

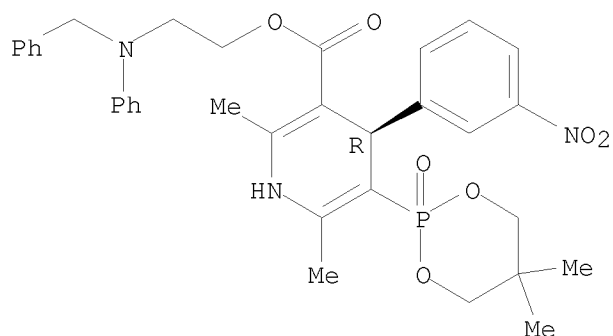


RN 128194-13-8 HCAPLUS

CN 3-Pyridinecarboxylic acid, 5-(5,5-dimethyl-2-oxido-1,3,2-dioxaphosphorinan-2-yl)-1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-, 2-[phenyl(phenylmethyl)amino]ethyl ester, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Updated Search



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 11:47:49 ON 04 MAR 2008)

FILE 'REGISTRY' ENTERED AT 11:48:44 ON 04 MAR 2008

L1 STRUCTURE UPLOADED
 L2 2 S L1
 L3 13 S L1 FULL
 L4 0 S L3 AND TAKADA, Y?/AU

FILE 'HCAPLUS' ENTERED AT 11:55:37 ON 04 MAR 2008

L5 180 S L3
 L6 10 S L3/PREP
 L7 1 S L6 AND TAKADA, Y?/AU

=> s l6 not l7

L8 9 L6 NOT L7

=> s l8 and matsumoto, h?/au

7407 MATSUMOTO, H?/AU
 L9 3 L8 AND MATSUMOTO, H?/AU

=> d l9, ibib abs hitstr, 1-3

L9 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:177130 HCAPLUS

DOCUMENT NUMBER: 139:307832

TITLE: Preparation of efonidipine hydrochloride as antihypertensive agent

AUTHOR(S): Matsumoto, Hiroo

CORPORATE SOURCE: Nissan Chemical Industries, Ltd., Japan

SOURCE: Purosesu Kemisutori no Shintenkai (2003), 253-265.

Shi Emu Shi Shuppan: Tokyo, Japan.

CODEN: 69DQZN; ISBN: 4-88231-384-7

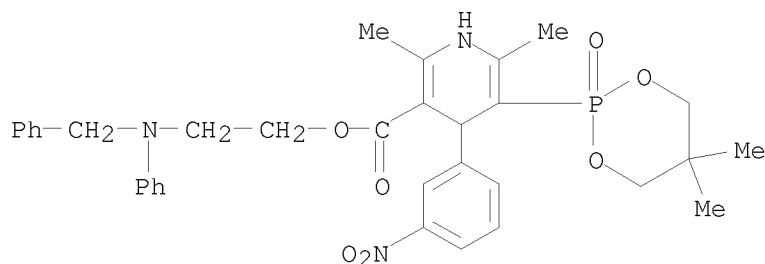
DOCUMENT TYPE: Conference; General Review

LANGUAGE: Japanese

AB A review on preparation of efonidipine hydrochloride as antihypertensive agent, covering new synthetic method for intermediate α -acetylstyrylphosphonate, determination of original drug, and preparation of optically

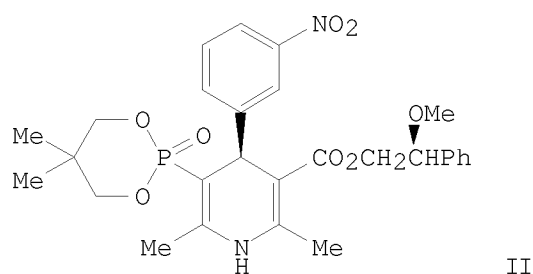
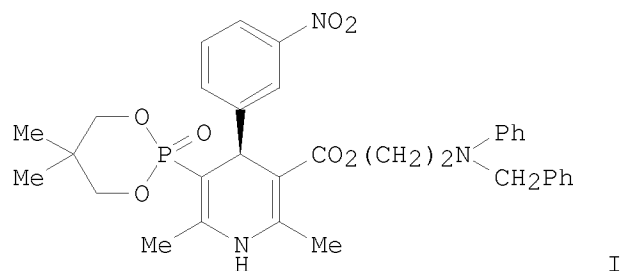
Updated Search

active isomer, etc.
 IT 111011-53-1P, Efonidipine hydrochloride
 RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of efonidipine hydrochloride as antihypertensive agent)
 RN 111011-53-1 HCAPLUS
 CN 3-Pyridinecarboxylic acid, 5-(5,5-dimethyl-2-oxido-1,3,2-dioxaphosphorinan-2-yl)-1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-, 2-[phenyl(phenylmethyl)amino]ethyl ester, hydrochloride (1:1) (CA INDEX NAME)



● HCl

L9 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1993:124669 HCAPLUS
 DOCUMENT NUMBER: 118:124669
 TITLE: Synthesis and crystal structure of optically active 2-[benzyl(phenyl)amino]ethyl 5-(5,5-dimethyl-2-oxo-1,3,2-dioxaphosphorinan-2-yl)-1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-3-pyridinecarboxylate (NZ-105)
 AUTHOR(S): Sakoda, Ryozo; Matsumoto, Hiroo; Seto, Kiyotomo
 CORPORATE SOURCE: Cent. Res. Inst., Nissan Chem. Ind. Ltd., Funabashi, 274, Japan
 SOURCE: Chemical & Pharmaceutical Bulletin (1992), 40(9), 2377-81
 CODEN: CPBTAL; ISSN: 0009-2363
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 118:124669
 GI



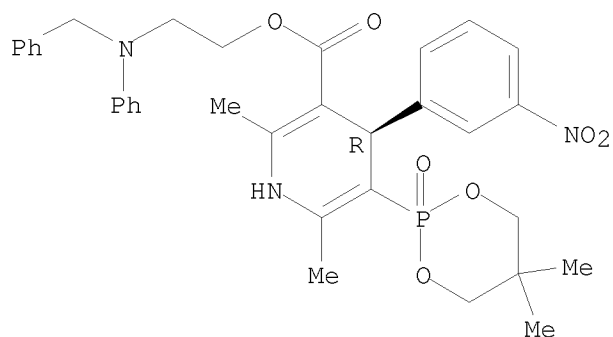
AB (S)-(Oxodioxaphosphorinanyl)(nitrophenyl)pyridinecarboxylate I ((S)-NZ-105) and the (R) isomer were synthesized through the fractional crystallization of (S)-Methoxyphenylethyl (oxodioxaphosphorinanyl)(nitrophenyl)pyridinecarboxylate II. Thus, II underwent N-methoxymethylation, transesterification, and demethoxymethylation to give I. The (R) isomer of II underwent the same treatment to give the (R) isomer of I. Calcium antagonism activity was found to reside in the S isomer from single crystal x-ray diffraction anal.

IT 128194-13-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and calcium antagonist activity of)

RN 128194-13-8 HCAPLUS

CN 3-Pyridinecarboxylic acid, 5-(5,5-dimethyl-2-oxido-1,3,2-dioxaphosphorinan-2-yl)-1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-, 2-[phenyl(phenylmethyl)amino]ethyl ester, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

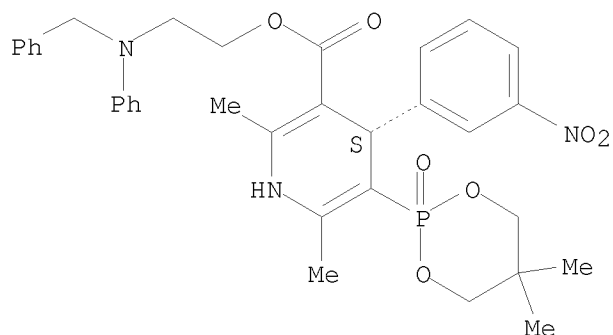


IT 128194-12-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)

Updated Search

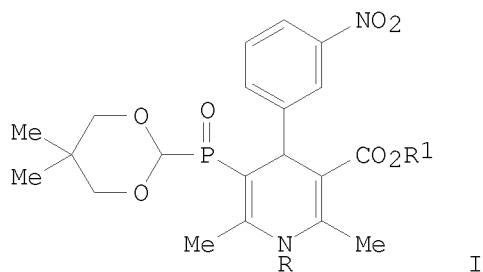
(preparation, crystal structure, and calcium antagonist activity of)
 RN 128194-12-7 HCAPLUS
 CN 3-Pyridinecarboxylic acid, 5-(5,5-dimethyl-2-oxido-1,3,2-dioxaphosphorinan-2-yl)-1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-, 2-[phenyl(phenylmethyl)amino]ethyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L9 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1990:459536 HCAPLUS
 DOCUMENT NUMBER: 113:59536
 TITLE: Preparation of optically active (dihydropyridyl)phosphonate esters as antihypertensives and their pharmaceutical compositions
 INVENTOR(S): Matsumoto, Hiroo; Kamikawa, Michimasaaki; Seto, Kyotomo; Sakota, Ryoza; Tanaka, Sakuya
 PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp. CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02011592	A	19900116	JP 1988-161909	19880629
PRIORITY APPLN. INFO.: GI			JP 1988-161909	19880629



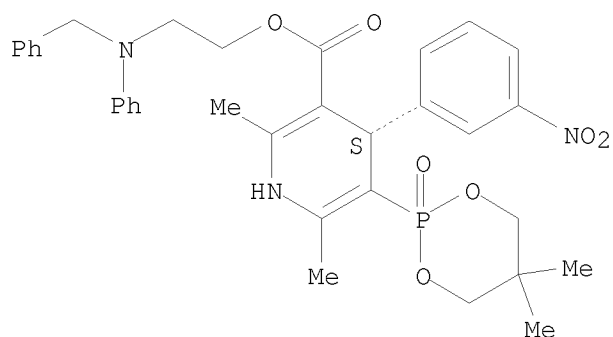
AB The title compds. (I; R = H, R1 = CH₂CH₂NPhCH₂Ph) (II), especially (S)-II, their pharmaceutically compatible salts and solvates, are prepared (S,S)-I (R = H, R1 = CH₂CHPhOMe) (preparation given) was stirred with 55% NaH in THF under cooling and then treated with ClCH₂OMe to give 73% methoxymethyl derivative (S,S)-I (R = MeOCH₂, R1 = CH₂CHPhOMe), which was treated with PhCH₂NPhCH₂CH₂ONa in C₆H₆ to give 45% (S)-I (R = MeOCH₂) (III). Hydrolysis of III with 28% HCl-EtOH gave 99% (S)-II, which showed -log(ID₅₀) of 8.86 as Ca antagonist in guinea pig. Also prepared and tested was (R)-II. Tablet, capsule, syrup, and powder formulations were given.

IT 128194-12-7P 128194-13-8P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of, as antihypertensive)

RN 128194-12-7 HCAPLUS

CN 3-Pyridinecarboxylic acid, 5-(5,5-dimethyl-2-oxido-1,3,2-dioxaphosphorinan-2-yl)-1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-, 2-[phenyl(phenylmethyl)amino]ethyl ester, (4S)- (9CI) (CA INDEX NAME)

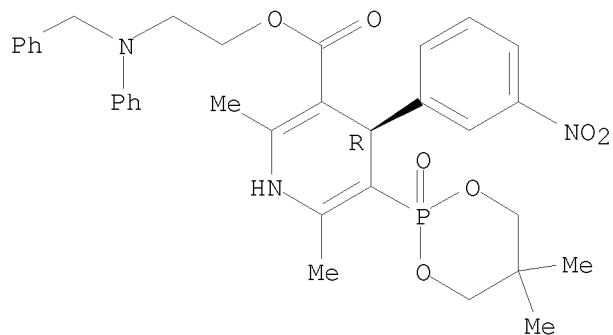
Absolute stereochemistry. Rotation (+).



RN 128194-13-8 HCAPLUS

CN 3-Pyridinecarboxylic acid, 5-(5,5-dimethyl-2-oxido-1,3,2-dioxaphosphorinan-2-yl)-1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-, 2-[phenyl(phenylmethyl)amino]ethyl ester, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



=> d his

(FILE 'HOME' ENTERED AT 11:47:49 ON 04 MAR 2008)

FILE 'REGISTRY' ENTERED AT 11:48:44 ON 04 MAR 2008

L1 STRUCTURE UPLOADED
L2 2 S L1
L3 13 S L1 FULL
L4 0 S L3 AND TAKADA, Y?/AU

FILE 'HCAPLUS' ENTERED AT 11:55:37 ON 04 MAR 2008

L5 180 S L3
L6 10 S L3/PREP
L7 1 S L6 AND TAKADA, Y?/AU
L8 9 S L6 NOT L7
L9 3 S L8 AND MATSUMOTO, H?/AU

=> s l8 not l9

L10 6 L8 NOT L9

=> d l10, ibib abs hitstr, 1-6

L10 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:325198 HCAPLUS

DOCUMENT NUMBER: 125:86734

TITLE: Asymmetric synthesis of (S)-(+)- and (R)-(-)-NZ-105
through the modified Michaelis-Arbuzov rearrangement
as a key step

AUTHOR(S): Kato, Tatsuhisa; Tejima, Mamiko; Ebiike, Hiroto;
Achiwa, Kazuo

CORPORATE SOURCE: School Pharmaceutical Sciences, University Shizuoka,
Shizuoka, 422, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1996), 44(5),
1132-1134

CODEN: CPBTAL; ISSN: 0009-2363

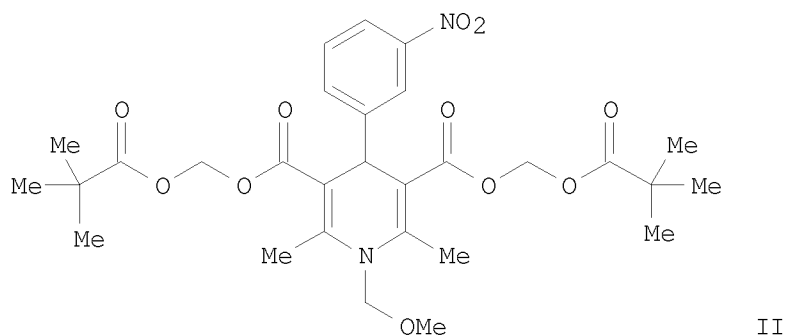
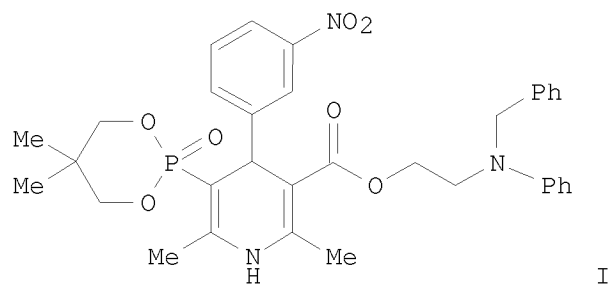
PUBLISHER: Pharmaceutical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 125:86734

GI



AB The asym. synthesis of the (S)-(+)- and (R)-(-)-NZ-105 (I) from the prochiral pyridine compound II was realized via a modified Hunsdiecker reaction followed by the modified Michaelis-Arbuzov reaction with zero valent palladium.

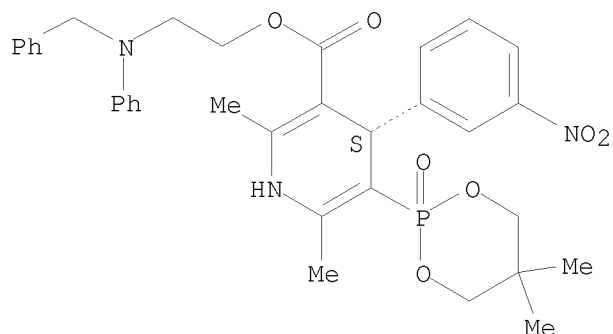
IT 128194-12-7P 128194-13-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. synthesis of NZ-105)

RN 128194-12-7 HCAPLUS

CN 3-Pyridinecarboxylic acid, 5-(5,5-dimethyl-2-oxido-1,3,2-dioxaphosphorinan-2-yl)-1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-, 2-[phenyl(phenylmethyl)amino]ethyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

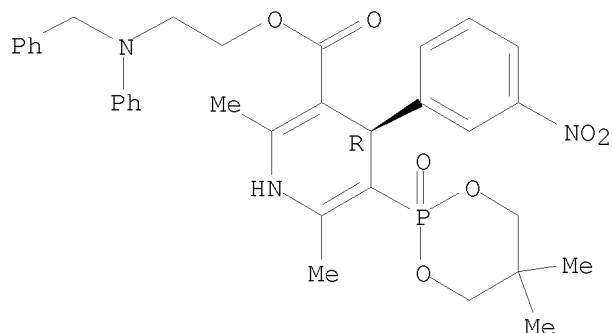


RN 128194-13-8 HCAPLUS

CN 3-Pyridinecarboxylic acid, 5-(5,5-dimethyl-2-oxido-1,3,2-dioxaphosphorinan-2-yl)-1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-, 2-[phenyl(phenylmethyl)amino]ethyl ester, (4R)- (9CI) (CA INDEX NAME)

Updated Search

Absolute stereochemistry. Rotation (-).



L10 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:772416 HCAPLUS

DOCUMENT NUMBER: 123:340043

TITLE: Lipase-catalyzed enantioselective synthesis of (R)- and (S)-2-[benzyl(phenyl)amino]ethyl 5-(5,5-dimethyl-2-oxo-1,3,2-dioxaphosphorinan-2-yl)-1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-3-pyridinecarboxylate (NZ 105)

AUTHOR(S): Ebiike, Hirosato; Yamazaki, Yukiyo; Achiwa, Kazuo
CORPORATE SOURCE: Sch. Pharm. Sci., Univ. Shizuoka, Shizuoka, 422, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1995), 43(7), 1251-3

CODEN: CPBTAL; ISSN: 0009-2363

PUBLISHER: Pharmaceutical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 123:340043

AB Optically active NZ 105 was smoothly prepared by enantioselective hydrolysis of the propionyloxymethyl ester by lipase and following esterification.

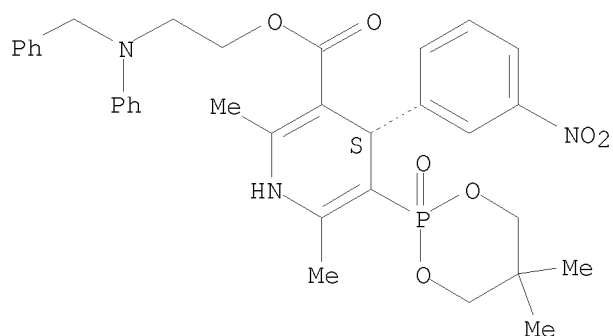
IT 128194-12-7P 128194-13-8P

RL: BPN (Biosynthetic preparation); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(lipase-catalyzed enantioselective preparation of NZ 105)

RN 128194-12-7 HCAPLUS

CN 3-Pyridinecarboxylic acid, 5-(5,5-dimethyl-2-oxido-1,3,2-dioxaphosphorinan-2-yl)-1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-, 2-[phenyl(phenylmethyl)amino]ethyl ester, (4S)- (9CI) (CA INDEX NAME)

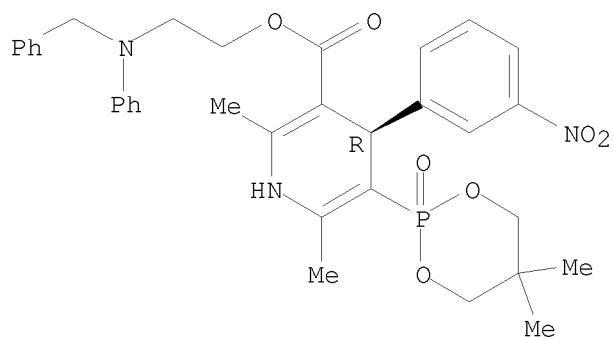
Absolute stereochemistry. Rotation (+).



RN 128194-13-8 HCAPLUS

CN 3-Pyridinecarboxylic acid, 5-(5,5-dimethyl-2-oxido-1,3,2-dioxaphosphorinan-2-yl)-1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-, 2-[phenyl(phenylmethyl)amino]ethyl ester, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L10 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:440280 HCAPLUS

DOCUMENT NUMBER: 123:9302

TITLE: Transformation of 1,4-dihydropyridine ring of calcium antagonist NZ-105 into cyclohexenone ring

AUTHOR(S): Kamikawaji, Yoshimasa; Sakoda, Ryo; Seto, Kiyotomo

CORPORATE SOURCE: Central Res. Inst., Nissan Chem. Industries, Ltd., Chiba, 274, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1995), 43(2), 315-17

CODEN: CPBTAL; ISSN: 0009-2363

PUBLISHER: Pharmaceutical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

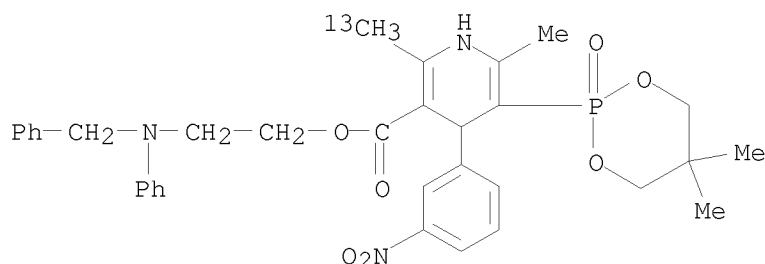
OTHER SOURCE(S): CASREACT 123:9302

AB On hydrolysis of the calcium antagonist, 2-(N-benzyl-N-phenylamino)ethyl 5-(5,5-dimethyl-2-oxo-1,3,2-dioxaphosphorinan-2-yl)-1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)pyridine-3-carboxylate hydrochloride ethanol (NZ-105 1.HCl.EtOH) in 35% hydrochloric acid, the 1,4-dihydropyridine ring was transformed to a cyclohexenone ring, affording cyclohexenone phosphonates.

IT 163808-73-9P

Updated Search

RN	163808-73-9	HCAPLUS
CN	3-Pyridinecarboxylic acid, 5-(5,5-dimethyl-2-oxido-1,3,2-dioxaphosphorinan-2-yl)-1,4-dihydro-6-methyl-2-(methyl-13C)-4-(3-nitrophenyl)-, 2-[phenyl(phenylmethyl)amino]ethyl ester (9CI) (CA INDEX NAME)	



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L10 ANSWER 4 OF 6      HCAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:      1993:124668  HCAPLUS
DOCUMENT NUMBER:       118:124668
TITLE:                 Synthesis of 1,4-dihydropyridine-5-phosphonates and
                        their calcium-antagonistic and antihypertensive
                        activities: novel calcium-antagonist
                        2-[benzyl(phenyl)amino]ethyl 5-(5,5-dimethyl-2-oxo-
                        1,3,2-dioxaphosphorinan-2-yl)-1,4-dihydro-2,6-dimethyl-
                        4-(3-nitrophenyl)-3-pyridinecarboxylate hydrochloride
                        ethanol (NZ-105) and its crystal structure
AUTHOR(S):             Sakoda, Ryozi; Kamikawaji, Yoshimasa; Seto, Kiyotomo
CORPORATE SOURCE:      Cent. Res. Inst., Nissan Chem. Ind. Co., Ltd.,
                        Funabashi, 274, Japan
SOURCE:                Chemical & Pharmaceutical Bulletin (1992), 40(9),
                        2362-9
                        CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE:         Journal
LANGUAGE:              English
OTHER SOURCE(S):       CASREACT 118:124668
GI
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The effect of the 3-carboxylic ester variation in 2,2-dimethyltrimethylene 3-alkoxycarbonyl-4-aryl-1,4-dihydro-2,6-dimethyl-5-pyridinephosphonates, e.g., I (R = 3-NO₂, 3-Cl, 2-OCHF₂, 2-CF₃) and II [R₁ = Me, Me₂CH, hexyl, octyl, nonyl, decyl, dodecyl, (CH₂)₆NMeCH₂Ph, (CH₂)₂NPhCH₂Ph, (CH₂)₂N(CH₂Ph)₂, Q, Q₁], was investigated in relation to the calcium-antagonistic and antihypertensive activities: the analogs containing the alkyl groups of not more than 12 carbons and an amino functionality in the carboxylic-ester moiety were synthesized to be examined for biol. activities. Among them, 2-[benzyl(phenyl)amino]ethyl 5-(5,5-dimethyl-2-oxo-1,3,2-dioxaphosphorinan-2-yl)-1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-3-pyridinecarboxylate hydrochloride ethanol (III) (NZ-105) showed particularly beneficial activities and was selected for further

pharmacol. studies and clin. development. Some aspects of the structure-activity relationships and solid-state structure of NZ-105 by x-ray crystallog. anal. are described.

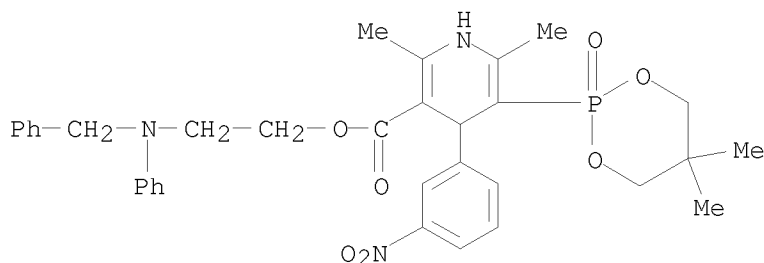
IT 111011-53-1P 111011-63-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and calcium antagonistic and hypertensive activity of)

RN 111011-53-1 HCAPLUS

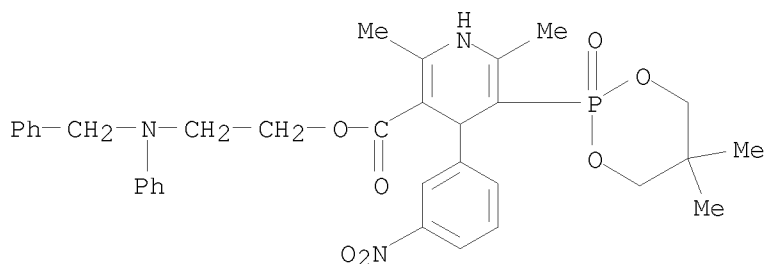
CN 3-Pyridinecarboxylic acid, 5-(5,5-dimethyl-2-oxido-1,3,2-dioxaphosphorinan-2-yl)-1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-, 2-[phenyl(phenylmethyl)amino]ethyl ester, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 111011-63-3 HCAPLUS

CN 3-Pyridinecarboxylic acid, 5-(5,5-dimethyl-2-oxido-1,3,2-dioxaphosphorinan-2-yl)-1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-, 2-[phenyl(phenylmethyl)amino]ethyl ester (CA INDEX NAME)



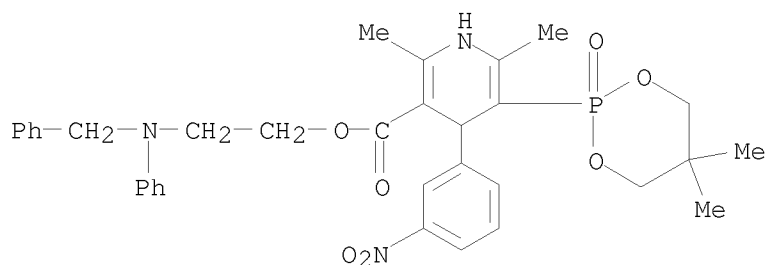
IT 146345-51-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation, crystal and mol. structure, and calcium antagonistic and antihypertensive activity of)

RN 146345-51-9 HCAPLUS

CN 3-Pyridinecarboxylic acid, 5-(5,5-dimethyl-2-oxido-1,3,2-dioxaphosphorinan-2-yl)-1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-, 2-[phenyl(phenylmethyl)amino]ethyl ester, monohydrochloride, monohydrate (9CI) (CA INDEX NAME)



● HCl

● H₂O

L10 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:538501 HCAPLUS

DOCUMENT NUMBER: 113:138501

TITLE: Pharmaceutical composition of dihydropyridine compound

INVENTOR(S): Miyajima, Masaharu; Yamaguchi, Yukiya; Tsunematsu, Takao; Oda, Toshihisa

PATENT ASSIGNEE(S): Zeria Pharmaceutical Co., Ltd., Japan; Nissan Chemical Industries, Ltd.

SOURCE: Eur. Pat. Appl., 10 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 344603	A1	19891206	EP 1989-109381	19890524
EP 344603	B1	19911023		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 02049728	A	19900220	JP 1989-50471	19890302
JP 2528706	B2	19960828		
AT 68699	T	19911115	AT 1989-109381	19890524
ES 2051920	T3	19940701	ES 1989-109381	19890524
CA 1332152	C	19940927	CA 1989-600631	19890525
US 4983593	A	19910108	US 1989-358144	19890530
PRIORITY APPLN. INFO.:			JP 1988-132262	A 19880530
			JP 1989-50471	A 19890302
			EP 1989-109381	A 19890524

OTHER SOURCE(S): CASREACT 113:138501

AB 5-(5,5-Dimethyl-1,3,2-dioxaphosphorinane-2-yl)-1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-3-pyridine carboxylic acid 2-[phenyl-(phenylmethyl)amino]ethyl ester P-oxide.HCl.ethanol solvate (1:1) (I) possessing hypotensive activity, is formulated with hydroxypropyl Me cellulose acetate succinate (II) to improve the water-solubility I 4 and II 12 g were dissolved into 100 mL of EtOH-CH₂Cl₂ (1:4) and 30 g lactose was added to the mixture The whole was dried and pulverized; the powder 23 g

was mixed with corn starch 10.7 g and talc 0.3 g and filled into capsules (total 340 mg/capsule or 20 mg I/capsule). A dissoln. test (according to Japanese Pharmacopeia) of the above capsules resulted in higher dissoln. rate than control capsules using other polymeric compds. instead of II. Also, in vivo studies with beagle dogs showed that the capsules provided an enhanced bioavailability.

IT 111011-76-8P, NZ 105 ethanolate

RL: PREP (Preparation)

(preparation of, capsules containing hydroxypropyl Me cellulose acetate succinate and, for water-solubility enhancement)

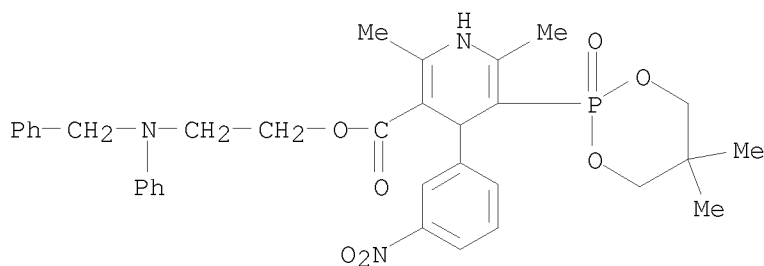
RN 111011-76-8 HCAPLUS

CN 3-Pyridinecarboxylic acid, 5-(5,5-dimethyl-2-oxido-1,3,2-dioxaphosphorinan-2-yl)-1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-, 2-[phenyl(phenylmethyl)amino]ethyl ester, monohydrochloride, compd. with ethanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 111011-53-1

CMF C34 H38 N3 O7 P . Cl H



● HCl

CM 2

CRN 64-17-5

CMF C2 H6 O

H₃C-CH₂-OH

L10 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1987:637009 HCAPLUS

DOCUMENT NUMBER: 107:237009

TITLE: Preparation of dihydropyridine-5-phosphonic acid cyclic propylene esters as antihypertensives and vasodilators

INVENTOR(S): Seto, Kiyotomo; Tanaka, Sakuya; Sakoda, Ryoza; Sakai, Tosinori; Masuda, Yukinori

PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan

Updated Search

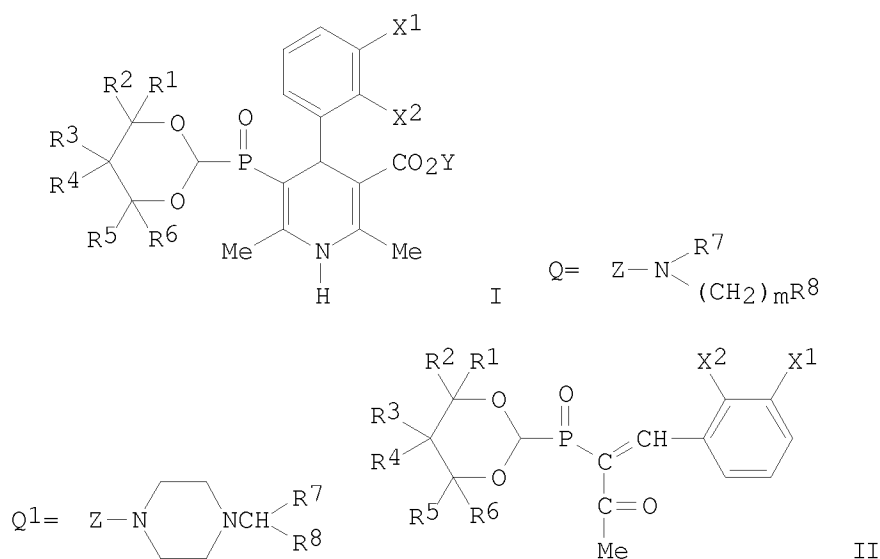
SOURCE: Eur. Pat. Appl., 28 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 6
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 230944	A1	19870805	EP 1987-100602	19870119
EP 230944	B1	19900207		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 62169795	A	19870725	JP 1986-11255	19860122
JP 06055751	B	19940727		
US 4885284	A	19891205	US 1986-851158	19860414
CA 1304379	C	19920630	CA 1986-507085	19860418
CN 87100286	A	19880113	CN 1987-100286	19870114
CN 1016063	B	19920401		
AU 8767635	A	19870723	AU 1987-67635	19870116
AU 589485	B2	19891012		
AT 50263	T	19900215	AT 1987-100602	19870119
WO 8704439	A1	19870730	WO 1987-JP32	19870120
W: BG, BR, DK, FI, HU, KR, NO, RO, SU				
ZA 8700403	A	19870930	ZA 1987-403	19870120
HU 44570	A2	19880328	HU 1987-768	19870120
HU 196605	B	19881228		
JP 63233992	A	19880929	JP 1987-10230	19870120
JP 06099458	B	19941207		
IL 81315	A	19911121	IL 1987-81315	19870120
DD 276873	A5	19900314	DD 1987-299387	19870121
FI 8703503	A	19870812	FI 1987-3503	19870812
FI 85491	B	19920115		
FI 85491	C	19920427		
SU 1586519	A3	19900815	SU 1987-4203193	19870814
DK 8704280	A	19870817	DK 1987-4280	19870817
DK 168821	B1	19940620		
NO 8703453	A	19870817	NO 1987-3453	19870817
NO 170728	B	19920817		
NO 170728	C	19921125		

PRIORITY APPLN. INFO.:

	JP 1986-11255	A	19860122
	JP 1986-12755	A	19860123
	US 1986-851158	A	19860414
	JP 1986-280159	A	19861125
	EP 1987-100602	A	19870119
	WO 1987-JP32	W	19870120

OTHER SOURCE(S): CASREACT 107:237009; MARPAT 107:237009
 GI



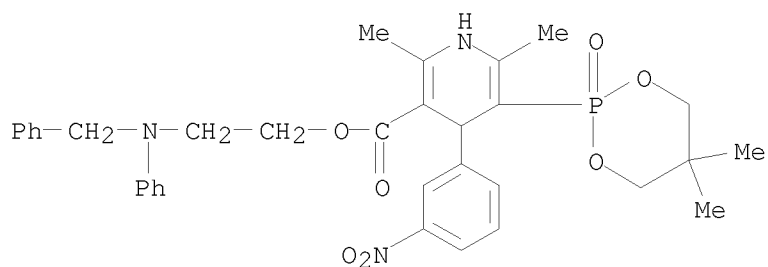
AB Title compds. I and their pharmaceutically acceptable salts (R1-R6 = H, C1-4 alkyl; one of X1, X2 = NO₂, F, Cl, OCHF₂, CF₃ and other is H; or X1 = X2 = Cl; Y = Q, Q1; Z = C2-6 alkylene; R7, R8 = chloro-, fluoro-, or alkoxyphenyl; m = 0-4) are prepared as vasodilators and antihypertensives. Refluxing a PhMe solution of 13.4 g 2-(N-benzyl-N-phenylamino)ethyl 3-aminocrotonate and 14.7 g II (R1 = R2 = R5 = R6 = H, R3 = R4 = Me, X1 = NO₂, X2 = H) for 10 h gave I [R1 = R2 = R5 = R6 = X2 = H, R3 = R4 = Me, X1 = NO₂, Y = CH₂CH₂N(Ph)(CH₂Ph)] (III). At 10 mg/kg oral with spontaneously hypertensive rats γ -III.HCl showed a slower onset and a longer lasting duration of action than Nicardipine.HCl. Tablets (1000) were formulated from γ -III.HCl 20.0, lactose 70.0, corn starch 25.0, cellulose 25.0, polyvinylpyrrolidone 8.0, and Mg stearate 2.0 g.

IT 111011-53-1P 111011-63-3P 111011-75-7P
111011-76-8P 111011-77-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as vasodilator and antihypertensive)

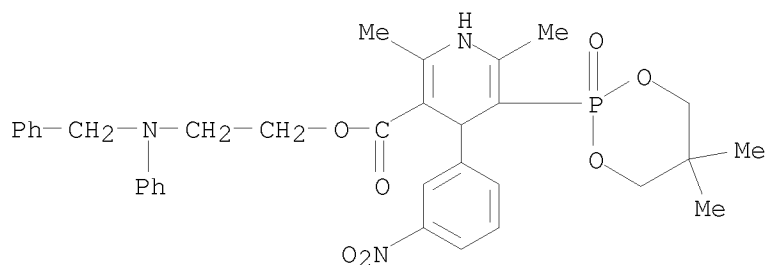
RN 111011-53-1 HCAPLUS

CN 3-Pyridinecarboxylic acid, 5-(5,5-dimethyl-2-oxido-1,3,2-dioxaphosphorinan-2-yl)-1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-, 2-[phenyl(phenylmethyl)amino]ethyl ester, hydrochloride (1:1) (CA INDEX NAME)



● HCl

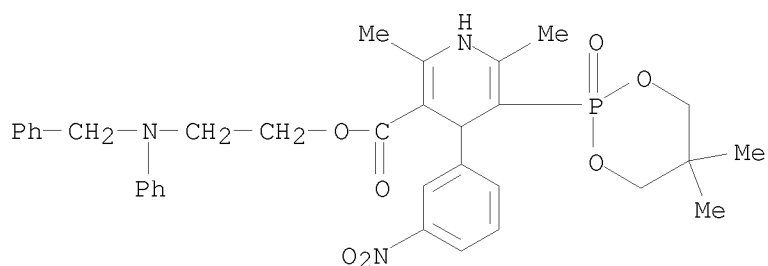
RN 111011-63-3 HCAPLUS
 CN 3-Pyridinecarboxylic acid, 5-(5,5-dimethyl-2-oxido-1,3,2-dioxaphosphorinan-2-yl)-1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-, 2-[phenyl(phenylmethyl)amino]ethyl ester (CA INDEX NAME)



RN 111011-75-7 HCAPLUS
 CN 3-Pyridinecarboxylic acid, 5-(5,5-dimethyl-2-oxido-1,3,2-dioxaphosphorinan-2-yl)-1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-, 2-[phenyl(phenylmethyl)amino]ethyl ester, compd. with methylbenzene (1:1) (9CI) (CA INDEX NAME)

CM 1

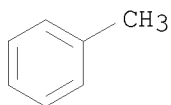
CRN 111011-63-3
 CMF C34 H38 N3 O7 P



CM 2

Updated Search

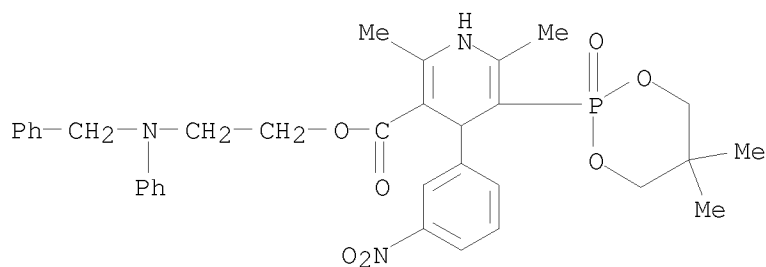
CRN 108-88-3
CMF C7 H8



RN 111011-76-8 HCAPLUS
CN 3-Pyridinecarboxylic acid, 5-(5,5-dimethyl-2-oxido-1,3,2-dioxaphosphorinan-2-yl)-1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-, 2-[phenyl(phenylmethyl)amino]ethyl ester, monohydrochloride, compd. with ethanol (1:1) (9CI) (CA INDEX NAME)

CM 1

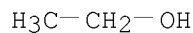
CRN 111011-53-1
CMF C34 H38 N3 O7 P . Cl H



● HCl

CM 2

CRN 64-17-5
CMF C2 H6 O



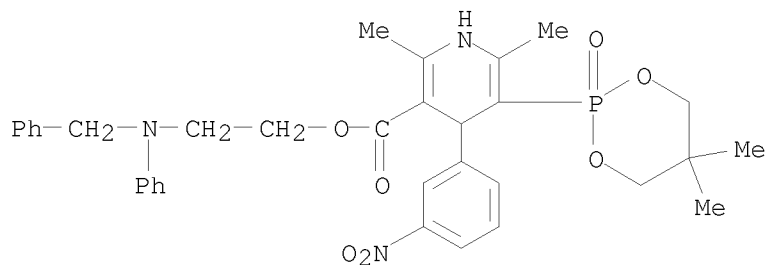
RN 111011-77-9 HCAPLUS
CN 3-Pyridinecarboxylic acid, 5-(5,5-dimethyl-2-oxido-1,3,2-dioxaphosphorinan-2-yl)-1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-, 2-[phenyl(phenylmethyl)amino]ethyl ester, monohydrochloride, compd. with acetonitrile (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 111011-63-3

Updated Search

CMF C34 H38 N3 O7 P



CM 2

CRN 75-05-8

CMF C2 H3 N

H₃C-C≡N

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COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

59.88

248.20

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

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-8.00

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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FILE 'REGISTRY' ENTERED AT 11:48:44 ON 04 MAR 2008

L1 STRUCTURE UPLOADED
L2 2 S L1
L3 13 S L1 FULL
L4 0 S L3 AND TAKADA, Y?/AU

FILE 'HCAPLUS' ENTERED AT 11:55:37 ON 04 MAR 2008

L5 180 S L3
L6 10 S L3/PREP
L7 1 S L6 AND TAKADA, Y?/AU
L8 9 S L6 NOT L7
L9 3 S L8 AND MATSUMOTO, H?/AU
L10 6 S L8 NOT L9

FILE 'CAOLD' ENTERED AT 11:56:59 ON 04 MAR 2008

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L11 0 L3